Dimethyl decanedioate

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Model Performance

Model Data	
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Weighted KNN model

5-fold CV (75%)		Training (75	Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.93	22.5	0.93	22.1	0.93	22.1	

Model Results

Predicted value: 272 °C

Global applicability domain: Inside

Local applicability domain index: 7.77e-01

Confidence level: 8.30e-01

Nearest Neighbors from the Training Set

Image not found

Dibutyl butanedioate Measured: 275 Predicted: 272 Image not found

Diethyl suberate Measured: 283 Predicted: 272 Image not found

Diisopentyl oxalate Measured: 268 Predicted: 258

Image not found

Diethyl isopentylmalonate

Measured: 241 Predicted: 258